Letters to the Editor

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DIMORPHISM OF DL-ASPARTIC ACID

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The occurrence of dimorphism in *DL*-aspartic acid has not been reported previously. The space group and a preliminary structure of this compound has been worked out by earlier workers (Dawson and Mathieson, 1951; Amirthalingam and Ramachandran, 1955) as $a = 9.18A.$, $b = 7.49A.$, $c = 15.79A.$, $\beta = 96°$, $Z = 8$ and the space group as $P2_1/a$. Pure *DL*-aspartic acid obtained from Nutritional Biochemicals Corporation Ltd., U.S.A., was crystallised from an aqueous solution at room temperature (34°C).

The spacings and $1/d^2$ values calculated from the powder patterns of the crystals of both the modifications are given in Table I. The visually estimated intensities of the reflections are given in parentheses as very strong (*vs*), strong (*s*), medium (*m*), weak (*w*) and very weak (*vw*).

The pattern of modification II was analysed by a modification of Lipson's method (1949) in which the $1/d^2$ values were used instead of the $\sin^2\theta$ values. The values of $1/d^2$ calculated after fixing the three constants $A(= 1/a^2,)$ $B(= 1/b^2)$ and $C\,(1/c^2)$ were compared with the observed values (Table I), within an accuracy of ± 0.0008.

Modification I

The values of $1/d^2$ calculated from the data of earlier workers agree reasonably well with the observed values of the present investigation (Table I). Hence the unit cell dimensions of the crystal of this modification are: $a = 9.18A.$, $b = 7.49A.$, $c = 15.79A.$, $\beta = 96°$ and $Z = 8$. The space group is $P2_1/a$.

Modification II

The crystal of this modification was found to belong to orthorhombic symmetry with the unit cell dimensions as $a = 15.00A.$, $b = 6.87A.$, $c = 10.26A.$, and $Z = 8$. The calculated density of 1.67 agrees very well with the accepted value of 1.663. The values of $1/d^2$ calculated from this data agree very well with the observed values as can be seen from Table I. The probable space group is $Pmmn(D^1_{2h})$.

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TABLE 1

Spacings and $1/d^2$ values of DL aspartic acid

Modification I				Modification II			
spacing in A. with intensity	values of I/d^2 obs.	values of I/d^2 calc.	indices	spacing in A. with intensity	values of I/d^2 obs.	values of I/d^2 calc.	indices
7.91 (w)	0.0160	0.0162	002	7.52 (w)	0.0177	0.0177	200
6.79 (vw)	0.0217	0.0218	011	5.11 (m)	0.0384	0.0380 0.0390	002 210
5.84 (vw)	0.0292	0.0298	110	4.10 (vs)	0.0596	0.0592	012
4.74 (vw)	0.0449	0.0431	$11\bar{2}$	3.95 (m)	0.0641	0.0635	112
4.59 (s)	0.0475	0.0483	200	3.78 (s)	0.0702	0.0707 0.0710	311 400
4.34 (vw)	0.0530	0.0542	013	3.51 (m)	0.0809	0.0806	401
3.95 (m)	0.0640	0.0648	004	3.42 (m)	0.0855	0.0848 0.0857	020 300
3.87 (w)	0.0667	0.0672	$21\bar{1}$	3.32 (w)	0.0902	0.0908	103
3.75 (ms)	0.0710	0.0707 0.0711	113 020	3.18 (s)	0.0988	0.0988 0.0993	121 312
3.40 (vs)	0.0867	0.0873	022	2.99 (vw)	0.1114	0.1111 0.1114 0.1122	500 113 221
3.27 (vw)	0.0934	0.0935 0.0938	203 $21\bar{3}$	2.89 (s)	0.1199	0.1194	501
3.15 (vw)	0.1013	0.1012 0.1015	005 $20\bar{4}$	2.80 (w)	0.1273	0.1279	122

TABLE I (*contd*).

modification I				modification II			
spacing in A. with intensity	values of I/d^2 obs.	calc.	indices	spacing in A. with intensity	values of I/d^2 obs.	calc.	indices
2.92 (m)	0.1170	0.1190	015	2.62 (m)	0.1462	0.1469	313
2.84 (w)	0.1240	0.1238 0.1240	$11\bar{5}$ 123	2.57 (m)	0.1518	0.1525	004
2.72 (w)	0.1350	0.1350 0.1359	$20\bar{5}$ 024	2.42 (s)	0.1702	0.1695 0 1703	601 204 ; 512
2.63 (w)	0.1438	0.1471	223	2.38 (w)	0.1770	0 1774	413
2.55 (m)	0.1538	0.1538	114	2.29 (m)	0.1913	0.1905 0.1915	611 214
2.46 (vw)	0.1649	0.1642 0.1647	031 ; 205 223	2.24 (w)	0.2003	0.2004 0.2009	031 700
2.41 (m)	0.1734	0.1721 0.1724	130 025				
2.36 (s)	0.1797	0.1795 0.1798	$32\bar{1}$ 320	2.19 (vw)	0.2085	0.2086	230
2.35 (s)	0.1815	0.1806	016	2.12 (vw)	0.2227	0.2222 0.2235	710 404
2.29 (w)	0.1910	0.1912 0.1915	132 401	2.08 (w)	0.2313	0.2310 0.2316	330 701
2.20 (w)	0.2050	0.2042 0.2058	$13\bar{3}$ 313				
2.16 (m)	0.2149	0.2153	231	2.06_5 (m)	0.2343	0.2340	522
2.11 (w)	0.2247	0.2263	$20\bar{7}$	2.05 (m)	0.2373	0.2373	024
2.05_6 (w)	0.2366	0.2360 0.2372	$23\bar{3}$ $12\bar{6}$	2.04 (m)	0.2396	0.2390 0.2403	702 331
2.01_6 (w)	0.2460	0.2473	403	1.99 (vw)	0.2533	0 2540	621
1.97 (w)	0.2569	0.2548	126	1.96 (vw)	0.2595	0.2593 0.2603	015 712
1.92_8 (vw)	0.2708	0.2714	$12\bar{7}$				
1.89_5 (vw)	0.2785	0.2772	331	1.92 (m)	0.2708	0.2713	413
1.87 (w)	0.2859	0.2848 0.2850	234 $21\bar{7}$	1.88_5 (m)	0.2814	0.2810 0.2816	133 523

TABLE I (*contd*).

modification I				modification II			
spacing in A. with intensity	values of I/d^2 obs.	values of I/d^2 calc.	indices	spacing in A. with intensity	values of I/d^2 obs.	values of I/d^2 calc.	indices
1.82_4 (w)	0.3007	0.2998 0.3007 0.3009	226 042 118	1.82 (m)	0.3021	0.3020	530
1.78 (w)	0.3173	0.3163	$32\bar{6}$	1.81 (m)	0.3050	0.3056	810
1.73_7 (vw)	0.3318	0.3307 0.3314	$12\bar{8}$ 511	1.76 (vw)	0.3236	0.3229 0.3238	025 722
1.71_8 (vw)	0.3388	0.3383 0.3397	227 $24\bar{1}$, $41\bar{6}$	1.71_5 (m)	0.3395	0.3393 0.3400	040 532
1.67_6 (m)	0.3560	0.3555 0.3556	$14\bar{4}$, $22\bar{5}$ 317	1.71 (m)	0.3425	0.3430	600
1.65 (vw)	0.3676	0.3672 0.3678	144 219	1.65_5 (m)	0.3647	0.3642	016
1.60 (m)	0.3879	0.3863 0.3876 0.3887	237 $52\bar{3}$ 236	1.64 (m)	0.3718	0.3715	723

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